Arbitrary Order Hierarchical Vector Bases for Hexahedrons

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1 Introduction

We present a clear and general method for constructing hierarchical vector bases of arbitrary polynomial degree for use in the finite element solution of Maxwell's equations. Our focus in this paper is on unstructured hexahedral grids with elements of higher order geometry (i.e. curved elements). Hierarchical bases enable p-refinement methods, where elements in a mesh can have different degrees of approximation, to be easily implemented. This can prove to be quite useful as sections of a computational domain can be selectively refined in order to achieve a greater error tolerance without the cost of refining the entire domain. In [1], hierarchical vector bases for tetrahedrons are presented up to degree 3. The tetrahedral bases presented in [2] are generalized for arbitrary polynomial degree. Here we present hierarchical vector bases of arbitrary polynomial degree for hexahedrons. We also present a systematic procedure for constructing the hierarchical degrees of freedom in terms of the well known interpolatory degrees of freedom. This procedure is not limited to hexahedrons, but can be applied to other topologies as well. Explicit degrees of freedom are required for any error analysis of a particular method and are necessary for applying Dirichlet boundary conditions to the surface of a mesh. In addition, the method presented here is unique in that the basis is computed only once on a reference element, then mapped to topologically equivalent elements of arbitrary order geometry using a set of well defined transformation rules. Recently, Hiptmair, motivated by the theory of exterior algebra and differential forms presented a unified mathematical framework for the construction of conforming finite element spaces [3]. In [3], both 1-form (also called $H(curl)$) and 2-form (also called $H(div)$) conforming finite element spaces and the definition of their degrees of freedom are presented. These degrees of freedom are weighted integrals where the weighting function determines the character of the bases, *i.e.* interpolatory, hierarchical, etc .... We demonstrate a set of hierarchical degrees of freedom that are consistent with this definition.

In this paper we follow the work of Ciarlet [4] and define a finite element as a set of three distinct objects $(\Omega, \mathcal{P}, \mathcal{A})$ such that:

- Ω is the polyhedral domain over which the element is defined
- $\mathcal{P}$ is a finite dimensional polynomial space from which basis functions are constructed
- $\mathcal{A}$ is a set of linear functionals (*Degrees of Freedom*) dual to $\mathcal{P}$

Finite element basis functions are *not* uniquely specified until all three components of $(\Omega, \mathcal{P}, \mathcal{A})$ are defined. The finite element basis functions, denoted as $\{\mathbf{w}\}$, are a particular basis of $\mathcal{P}$ implicitly defined by the relation

$$\mathcal{A}_i(\mathbf{w}_j) = \delta_{i,j} \tag{1}$$

We present a specific procedure for computing a hierarchical 1-form basis of arbitrary polynomial degree as well as the corresponding hierarchical degrees of freedom.

2 Polynomials

Both interpolatory and orthogonal polynomials will be the building blocks for the hierarchical basis functions. As such, we introduce two specific types of polynomials. The Lagrange interpolatory polynomial of degree p, which we will denote as $L_i^p(x)$, is defined by a distinct set of $p+1$ real valued interpolation points $\{X_j\} \in [0,1]$ for $j = 0, \ldots, p$. The polynomial is constructed in such a way that it has a value of unity at the $i'th$ interpolation point and a value of zero at every other interpolation point. In addition, we will use a variation of the Legendre polynomials defined over

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the reference segment $[0, 1]$, which we will denote as $\bar{l}^p(x)$, where p is the degree of the polynomial. Specifically, we have

$$L_i^p(x) = \prod_{\substack{j=0 \\ j \neq i}}^{p} \frac{(x - X_j)}{(X_i - X_j)}; \quad \bar{l}^p(x) = l^p(2x - 1), \tag{2}$$

where $l^p(x)$ is the standard definition of the Legendre polynomial of degree p defined over the segment $[-1, 1]$.

3 Ω - Element Topology and Geometry

We perform all computations on a reference element $\hat{\Omega}$ (all objects explicitly defined on the reference element will be accented with a *hat* symbol). All hexahedral elements (including curved elements) in a physical mesh are topologically equivalent to a reference element. There exists a mapping Φ from the reference element $\hat{\Omega}$ to the actual element Ω. This mapping (defined by interpolatory *shape functions*) and its Jacobian are defined as

$$\mathbf{x} = \Phi(\hat{\mathbf{x}}); \quad \mathbf{J}_{i,j} = \frac{\partial x_j}{\partial \hat{x}_i}, \tag{3}$$

where $\hat{\mathbf{x}} \in \hat{\Omega}$ and $\mathbf{x} \in \Omega$. Unlike the approaches presented in [1], [2] and[5], we define the basis functions $\hat{\mathbf{w}}$ on the reference element and transform them as necessary during the finite element assembly procedure. We do this because the hierarchical basis functions are expensive to compute; using the following transformations the bases need only be computed once. The appropriate transformations for 1-forms and their derivative are

$$\mathbf{w} = \mathbf{J}^{-1}(\hat{\mathbf{w}} \circ \Phi); \quad d\mathbf{w} = \frac{1}{|\mathbf{J}|}\mathbf{J}^T(d\hat{\mathbf{w}} \circ \Phi) \tag{4}$$

4 $\mathcal{P}$ - Polynomial Space

For $\mathcal{P}$ we use the polynomial space originally proposed in [6], which is valid for discretization of the space $H(curl)$. Let $Q_{p_1,p_2,\ldots,p_n}$ denote a polynomial of n variables $(x_1, x_2, \ldots, x_n)$ whose maximum degree is p_1 in x_1, p_2 in x_2, $\ldots$, p_n in x_n. Using this notation, the appropriate polynomial space for a 1-form basis on the unit hexahedron is

$$\mathcal{P}^p(\hat{\Omega}) = \{\mathbf{u}; u_x \in Q_{p-1,p,p}, u_y \in Q_{p,p-1,p}, u_z \in Q_{p,p,p-1}\}; \quad dim(\mathcal{P}^p(\hat{\Omega})) = 3p(p+1)^2 \tag{5}$$

Note that $\mathcal{P}^p(\hat{\Omega})$ does not yet define our finite element basis functions. The final hierarchical finite element basis functions are a particular basis of $\mathcal{P}^p(\hat{\Omega})$ defined by eq (1).

5 Basis Functions

In order to ensure the proper conformity across element to element interfaces, it is crucial that the basis functions (and consequently the degrees of freedom) be associated with the various sub-simplices of the element (e.g. edges, faces, etc $\ldots$). This implies that subsets of the basis will span corresponding subspaces of the polynomial space $\mathcal{P}$. If we denote a hierarchical basis on the reference element as $\hat{W}$, then for 1-forms, we can break this set of basis functions into three mutually disjoint subsets such that

$$\hat{W} = \hat{W}_e \cup \hat{W}_f \cup \hat{W}_v, \tag{6}$$

where the subscripts e, f and v denote the edges, faces and volume of the reference element. The edge basis functions of polynomial degree p are given by

$$\hat{W}_e = \begin{cases} L_i^1(y)L_j^1(z)\bar{l}^k(x)\hat{\mathbf{x}} \\ L_i^1(x)L_j^1(z)\bar{l}^k(y)\hat{\mathbf{y}} \\ L_i^1(x)L_j^1(y)\bar{l}^k(z)\hat{\mathbf{z}} \end{cases} \quad i, j = 0, 1; \quad k = 0, \ldots, p-1 \tag{7}$$

where $\hat{\mathbf{x}}, \hat{\mathbf{y}}$ and $\hat{\mathbf{z}}$ denote the standard Cartesian basis vectors. The indices i and j loop over the 4 edges that are tangent to these basis vectors. The index k loops over the p basis functions per edge The subset $\hat{W}_e$ spans the subspace $Q_{p-1,1,1} \oplus Q_{1,p-1,1} \oplus Q_{1,1,p-1}$, which has a dimension of $12p$. The face basis functions of polynomial degree p are given by

$$\hat{W}_f = \begin{cases} L_i^1(x)\bar{l}^j(y)\bar{l}^k(z)L_1^2(z)\hat{\mathbf{y}} \\ L_i^1(x)\bar{l}^j(z)\bar{l}^k(y)L_1^2(y)\hat{\mathbf{z}} \\ L_i^1(y)\bar{l}^j(x)\bar{l}^k(z)L_1^2(z)\hat{\mathbf{x}} \\ L_i^1(y)\bar{l}^j(z)\bar{l}^k(x)L_1^2(x)\hat{\mathbf{z}} \\ L_i^1(z)\bar{l}^j(x)\bar{l}^k(y)L_1^2(y)\hat{\mathbf{x}} \\ L_i^1(z)\bar{l}^j(y)\bar{l}^k(x)L_1^2(x)\hat{\mathbf{y}} \end{cases} \quad i = 0, 1; \;\; j = 0, \ldots, p-1; \;\; k = 0, \ldots, p-2 \tag{8}$$

This set of functions is grouped into 6 sub-sets, two for each face representing the basis vectors that are in the plane of that face. The index i loops over the 2 faces that are normal to these basis vectors. The indices j and k loop over the $2p(p-1)$ basis functions per face for a total of $12p(p-1)$. The subset $\hat{W}_f$ spans the subspace $Q_{1,p-1,p-2} \oplus Q_{1,p-2,p-1}$ for faces normal to the $\hat{\mathbf{x}}$ direction, $Q_{p-1,1,p-2} \oplus Q_{p-2,1,p-1}$ for faces normal to the $\hat{\mathbf{y}}$ direction and $Q_{p-1,p-2,1} \oplus Q_{p-2,p-1,1}$ for faces normal to the $\hat{\mathbf{z}}$ direction. Finally, there will be a total of $3p(p-1)^2$ basis functions that are internal to the reference element (i.e. functions not shared between elements), given by

$$\hat{W}_v = \begin{cases} \bar{l}^i(y)L_1^2(y)\bar{l}^j(z)L_1^2(z)\bar{l}^k(x)\hat{\mathbf{x}} \\ \bar{l}^i(x)L_1^2(x)\bar{l}^j(z)L_1^2(z)\bar{l}^k(y)\hat{\mathbf{y}} \\ \bar{l}^i(x)L_1^2(x)\bar{l}^j(y)L_1^2(y)\bar{l}^k(z)\hat{\mathbf{z}} \end{cases} \quad i, j = 0, \ldots, p-2; \;\; k = 0, \ldots, p-1 \tag{9}$$

The subset $\hat{W}_v$ spans the subspace $Q_{p-1,p-2,p-2} \oplus Q_{p-2,p-1,p-2} \oplus Q_{p-2,p-2,p-1}$.

It is important to point out that, by construction, the basis functions associated with a given sub-simplex are all orthogonal to each other. For example, all basis functions associated with a given edge are mutually orthogonal, while all of the volume (or interior) basis functions are mutually orthogonal.

6 $\mathcal{A}$ - Degrees of Freedom

The set $\mathcal{A}$ of degrees of freedom consists of linear functionals that map an arbitrary function, $\mathbf{g}$, onto the set of real numbers. The set $\mathcal{A}$ satisfies three important properties; namely

- *Unisolvence*: $\mathcal{A}$ is dual to the finite element space, *i.e.* eq (1) must hold.
- *Invariance*: Degrees of freedom remain unisolvent upon a change of variables.
- *Locality*: The trace of a basis function on a sub-simplex is determined by degrees of freedom associated *only* with that sub-simplex.

The degrees of freedom are best understood in the following context. Suppose we have a 1-form field (for example, the 1-form electric field) that we wish to approximate using a vector basis function expansion. The expansion would be of the form

$$\mathbf{g} \approx \sum_{i=1}^{dim(W)} \mathcal{A}_i(\mathbf{g})\mathbf{w}_i \tag{10}$$

The degrees of freedom act as weights in the expansion and are computed by *projecting* the function $\mathbf{g}$ onto the dual space spanned by $\mathcal{A}$ in a manner completely analogous to computing the coefficients in a Fourier expansion. This projection operation is required by finite element simulation codes to implement source terms, boundary conditions, etc ....

Given the previously defined hierarchical basis functions, we can construct a hierarchical set of degrees of freedom in a fairly simple manner. The key lies in the definition of the unisolvence property in eq (1) and the fact that the polynomial space $\mathcal{P}$ and the degrees of freedom $\mathcal{A}$ are dual to each other. Because the functionals from $\mathcal{A}$ are linear, we can form a new set by taking a linear combination of any previously valid set and then imposing the unisolvence requirement. Consider the well known and easy to construct interpolatory 1-form degrees of freedom

$$\mathcal{A}_i^I(\mathbf{g}) = \mathbf{g}(\Phi(x_i)) \cdot \mathbf{J}^T(\vec{\mathbf{t}}_i), \tag{11}$$

where x_i is a particular interpolation point in the reference coordinate system and $\vec{\mathbf{t}}_i$ is an edge tangent vector associated with the point x_i. Now we apply these degrees of freedom to our hierarchical basis and construct the matrix

$$V_{i,j} = \mathcal{A}_i^I(\hat{\mathbf{w}}_j); \quad \hat{\mathbf{w}}_j \in \hat{W} \tag{12}$$

The new hierarchical degrees of freedom, denoted $\mathcal{A}^H$, are then defined in terms of this transformation matrix and the interpolatory degrees of freedom by

$$\mathcal{A}^H = (V^{-1})^T \mathcal{A}^I \tag{13}$$

In [6], the degrees of freedom are given by the following *weighted* moment integrals

$$\begin{aligned}
\mathcal{A}^e(\mathbf{g}) &= \int_{\hat{e}} (\mathbf{g} \circ \Phi) \cdot \mathbf{J}^T(\vec{\mathbf{t}} q), \\
\mathcal{A}^f(\mathbf{g}) &= \iint_{\hat{f}} (\mathbf{g} \circ \Phi) \cdot \mathbf{J}^T(\vec{\mathbf{n}} \times \mathbf{q}), \\
\mathcal{A}^v(\mathbf{g}) &= \iiint_{\hat{v}} (\mathbf{g} \circ \Phi) \cdot \mathbf{J}^T \mathbf{q}
\end{aligned}$$

The hierarchical degrees of freedom given by eqs (12) and (13) are in fact discrete versions of these moment integrals. For example, hierarchical degrees of freedom on an edge are expressed as a weighted sum of interpolatory degrees of freedom associated with that edge only, while hierarchical degrees of freedom on a face are expressed as a weighted sum of interpolatory degrees of freedom associated with that face only. In addition, these degrees of freedom satisfy the commuting diagram property in a discrete sense.

7 Conclusions

Hierarchical basis functions are useful for several reasons. First, they provide a simple way of connecting elements of different degrees of approximation in a conforming manner, this is accomplished by discarding higher order terms on element sub-simplices. Secondly, if constructed properly the basis functions have maximum orthogonality, which is especially important for time domain problems where a linear system needs to be solved at every time step. We have presented a set of fully hierarchical 1-form basis functions and their corresponding degrees of freedom, suitable for discretization of the space $H(curl)$ on unstructured hexahedral meshes. In addition, a general procedure for computing hierarchical degrees of freedom using interpolatory degrees of freedom was presented.

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